

Data Path : Z:\HPCHEM1\BNA F\DATA\BF123016\  
 Data File : BF092044.D  
 Acq On : 30 Dec 2016 14:01  
 Operator : UM/SJ  
 Sample : H6262-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 W-4(55-57)

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 2.887       | 69            | 70          | 88           | rBV      | 69065          | 271383        | 3.45%           | 0.386%        |
| 2         | 4.830       | 237           | 240         | 250          | rBV      | 1206317        | 2126331       | 27.04%          | 3.026%        |
| 3         | 5.287       | 277           | 280         | 283          | rBV      | 4487280        | 6423594       | 81.69%          | 9.140%        |
| 4         | 6.350       | 369           | 373         | 375          | rBV      | 5734119        | 6836164       | 86.94%          | 9.727%        |
| 5         | 6.453       | 379           | 382         | 385          | rBV      | 5639865        | 6005742       | 76.38%          | 8.546%        |
| 6         | 6.682       | 399           | 402         | 404          | rBV      | 1282342        | 1247930       | 15.87%          | 1.776%        |
| 7         | 6.842       | 413           | 416         | 418          | rBV      | 4076184        | 5147908       | 65.47%          | 7.325%        |
| 8         | 7.253       | 448           | 452         | 454          | rBV      | 4242650        | 4787498       | 60.89%          | 6.812%        |
| 9         | 7.962       | 512           | 514         | 517          | rBV      | 1811448        | 1938803       | 24.66%          | 2.759%        |
| 10        | 9.048       | 606           | 609         | 611          | rBV      | 7325046        | 7863000       | 100.00%         | 11.189%       |
| 11        | 9.448       | 641           | 644         | 646          | rBV      | 2862535        | 2755867       | 35.05%          | 3.921%        |
| 12        | 9.653       | 657           | 662         | 665          | rBV2     | 109100         | 217869        | 2.77%           | 0.310%        |
| 13        | 9.710       | 665           | 667         | 670          | rBV      | 1723403        | 2163328       | 27.51%          | 3.078%        |
| 14        | 9.939       | 684           | 687         | 689          | rBV      | 79730          | 116296        | 1.48%           | 0.165%        |
| 15        | 10.156      | 701           | 706         | 710          | rVB3     | 77102          | 165888        | 2.11%           | 0.236%        |
| 16        | 10.511      | 733           | 737         | 739          | rBV      | 4172757        | 5146084       | 65.45%          | 7.323%        |
| 17        | 10.636      | 743           | 748         | 751          | rBV2     | 118707         | 238732        | 3.04%           | 0.340%        |
| 18        | 11.082      | 782           | 787         | 788          | rBV2     | 116669         | 159292        | 2.03%           | 0.227%        |
| 19        | 11.196      | 794           | 797         | 799          | rBV      | 2457250        | 2306950       | 29.34%          | 3.283%        |
| 20        | 11.505      | 822           | 824         | 827          | rVB      | 100638         | 94209         | 1.20%           | 0.134%        |
| 21        | 11.745      | 842           | 845         | 849          | rBV2     | 1014042        | 1305777       | 16.61%          | 1.858%        |
| 22        | 11.882      | 855           | 857         | 864          | rVB2     | 29438          | 87500         | 1.11%           | 0.125%        |
| 23        | 12.522      | 910           | 913         | 919          | rBV2     | 486022         | 818267        | 10.41%          | 1.164%        |
| 24        | 12.625      | 919           | 922         | 925          | rVB2     | 70589          | 124619        | 1.58%           | 0.177%        |
| 25        | 12.785      | 933           | 936         | 939          | rBV      | 6003286        | 6725808       | 85.54%          | 9.570%        |
| 26        | 13.345      | 981           | 985         | 988          | rBV3     | 47746          | 90501         | 1.15%           | 0.129%        |
| 27        | 13.688      | 1012          | 1015        | 1024         | rBV2     | 353051         | 477563        | 6.07%           | 0.680%        |
| 28        | 13.825      | 1024          | 1027        | 1030         | rBV      | 2282319        | 2248690       | 28.60%          | 3.200%        |
| 29        | 14.317      | 1066          | 1070        | 1076         | rBV2     | 53949          | 133046        | 1.69%           | 0.189%        |
| 30        | 14.911      | 1119          | 1122        | 1127         | rBV      | 84292          | 130330        | 1.66%           | 0.185%        |
| 31        | 15.208      | 1145          | 1148        | 1150         | rBV      | 1435246        | 1786930       | 22.73%          | 2.543%        |
| 32        | 15.631      | 1182          | 1185        | 1187         | rBV      | 94120          | 153937        | 1.96%           | 0.219%        |
| 33        | 16.065      | 1220          | 1223        | 1228         | rVB2     | 41695          | 91239         | 1.16%           | 0.130%        |
| 34        | 16.328      | 1242          | 1246        | 1251         | rVB2     | 44471          | 89723         | 1.14%           | 0.128%        |

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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

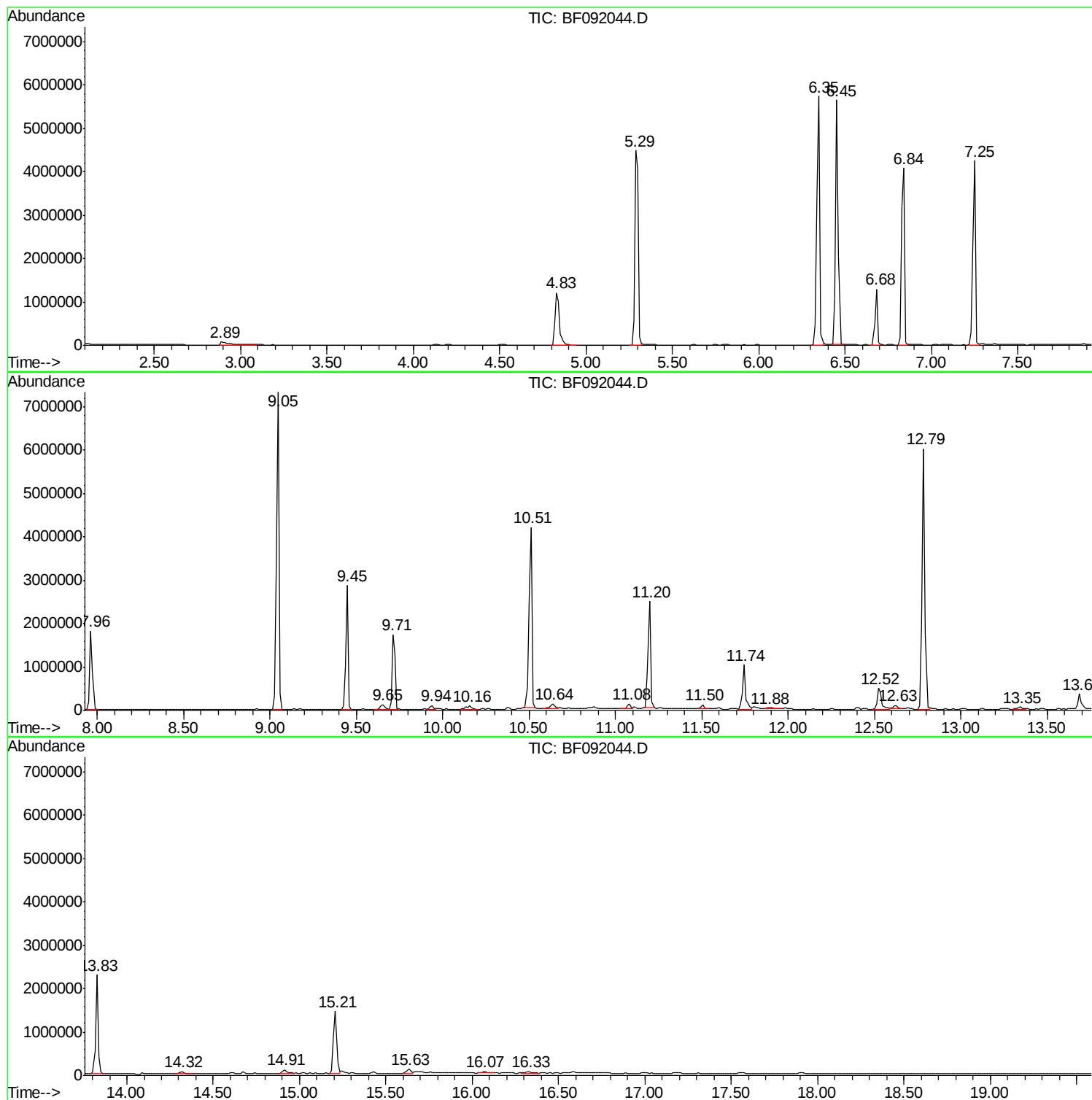
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

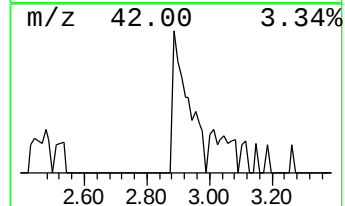
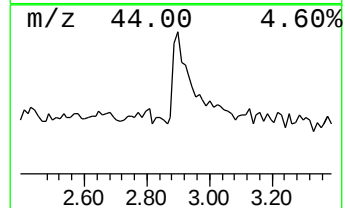
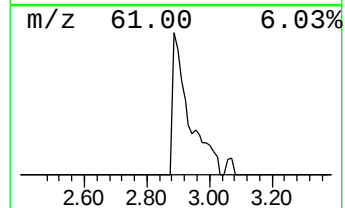
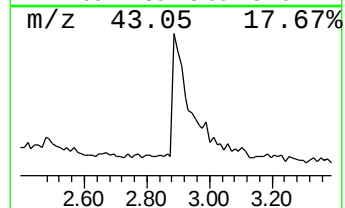
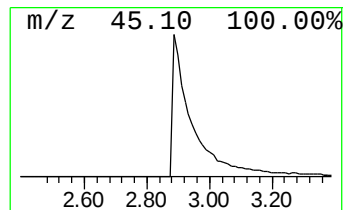
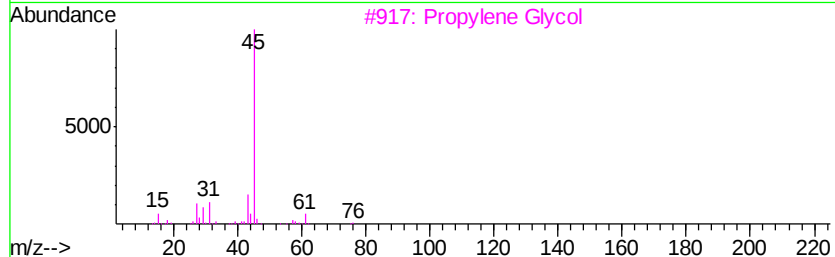
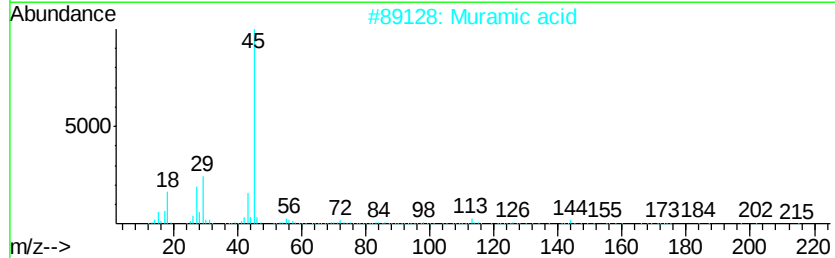
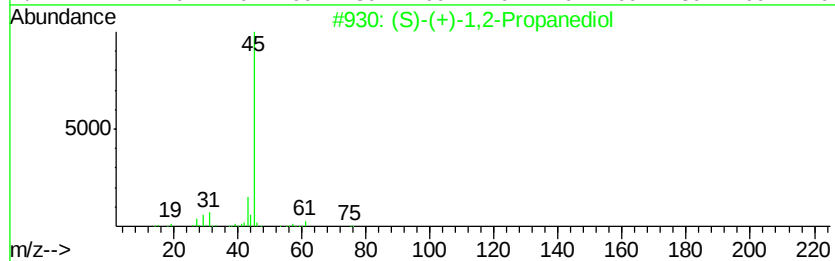
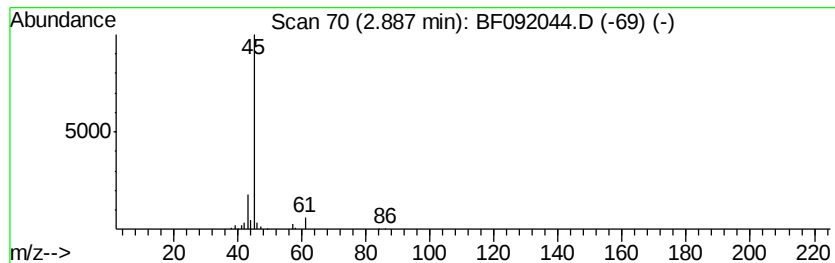
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.89 Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 2.89 | 4.35 ng | 271383 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | (S)-(+)-1,2-Propanediol             | 76  | C3H8O2   | 004254-15-3 | 40   |
| 2    |    | Muramic acid                        | 251 | C9H17NO7 | 001114-41-6 | 9    |
| 3    |    | Propylene Glycol                    | 76  | C3H8O2   | 000057-55-6 | 9    |
| 4    |    | Methyltartronic acid                | 134 | C4H6O5   | 000595-98-2 | 9    |
| 5    |    | Propanoic acid, 2-hydroxy-, meth... | 104 | C4H8O3   | 002155-30-8 | 9    |



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ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

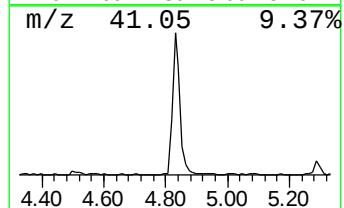
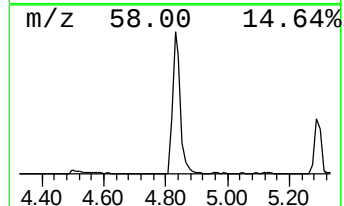
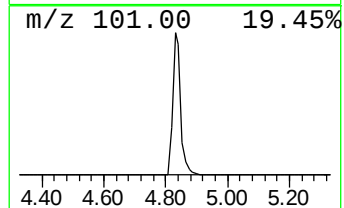
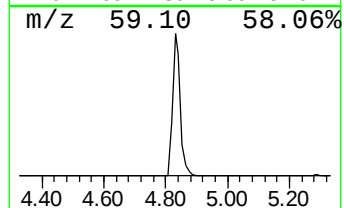
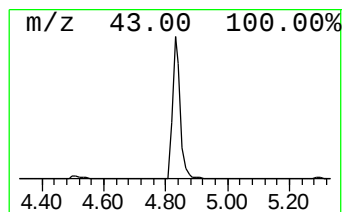
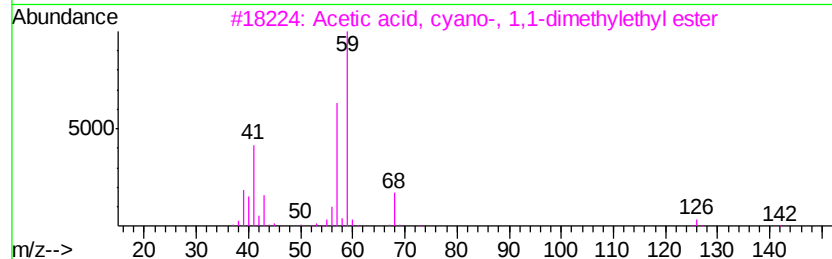
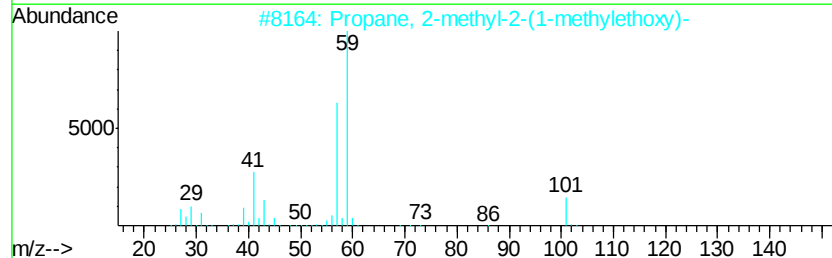
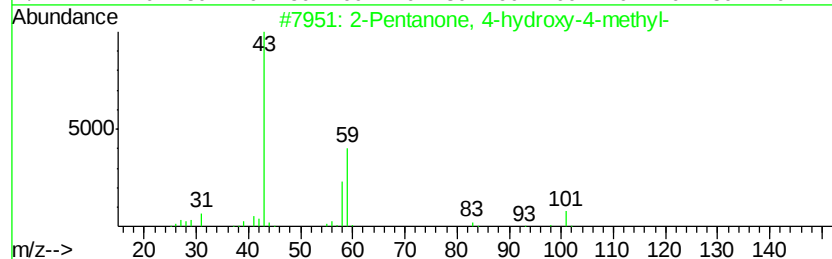
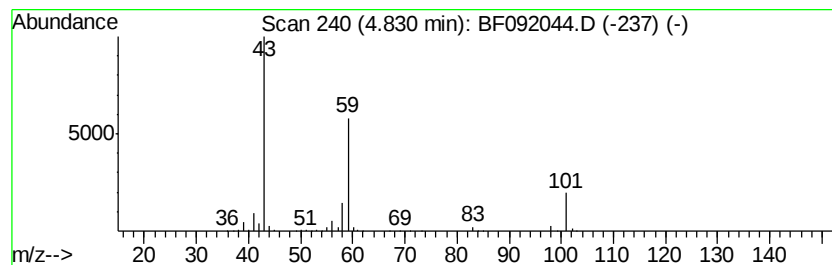
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.83 | 34.08 ng | 2126330 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                          | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-      | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Propane, 2-methyl-2-(1-methylethoxy)- | 116 | C7H16O   | 017348-59-3 | 42   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethyl-    | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    | Morpholine, 4-methyl-                 | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | 2,3-Butanedione, monooxime            | 101 | C4H7NO2  | 000057-71-6 | 9    |



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Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

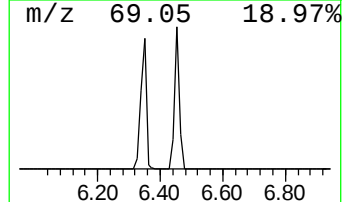
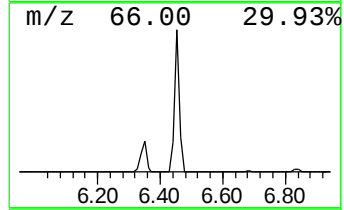
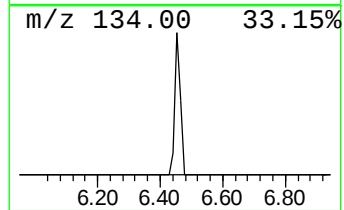
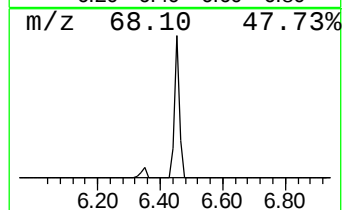
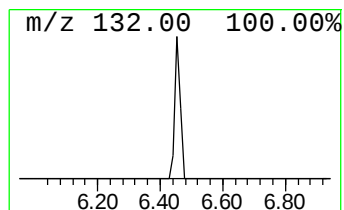
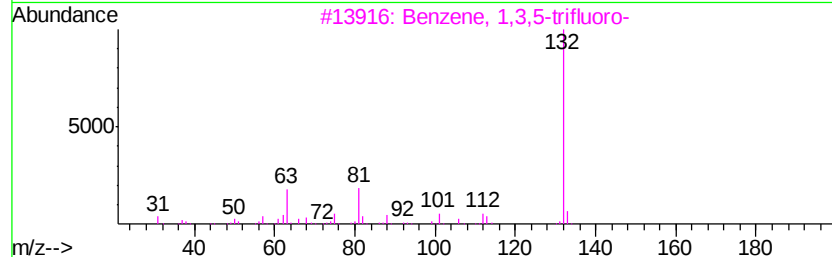
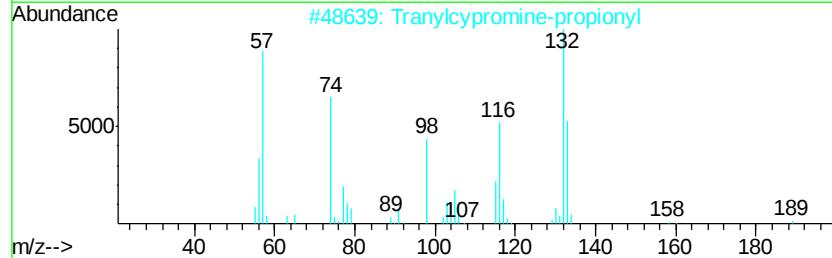
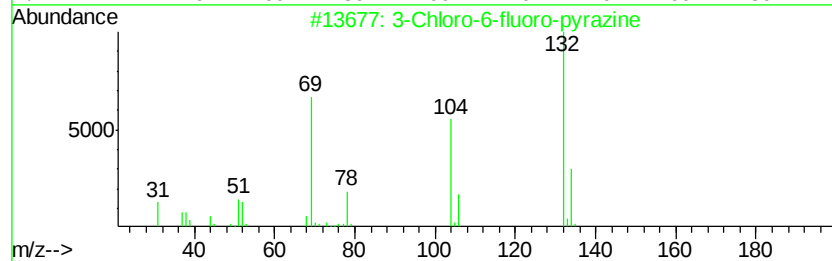
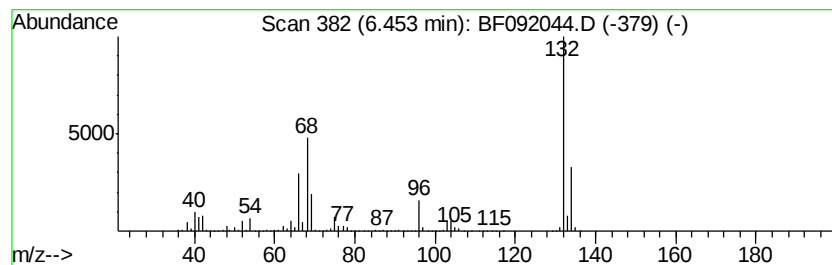
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown6.45 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.45 | 96.25 ng | 6005740 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    | Benzene, 1,3,5-trifluoro-           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 4    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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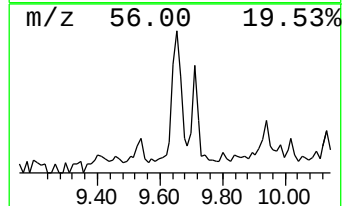
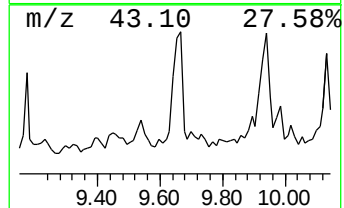
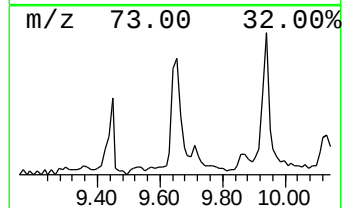
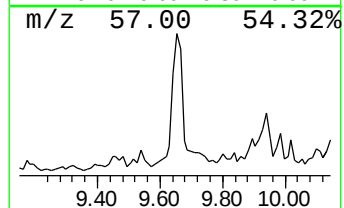
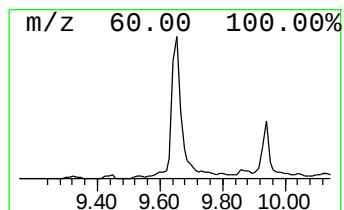
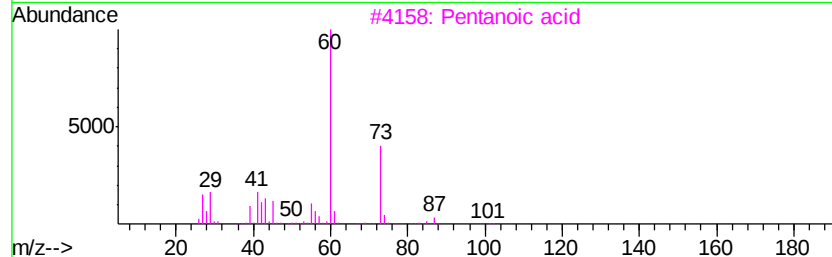
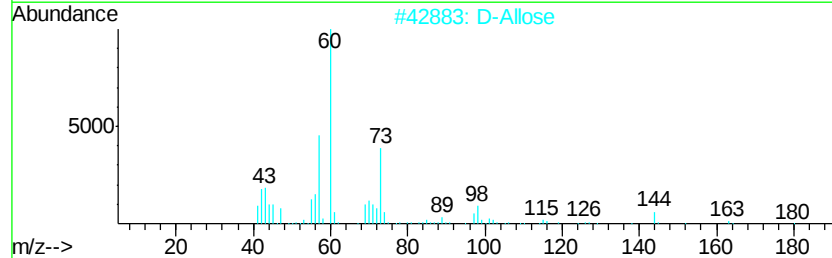
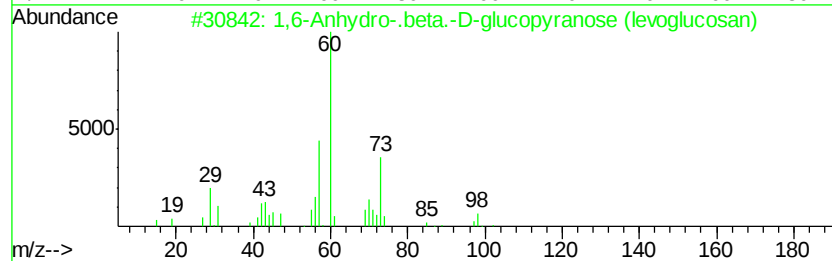
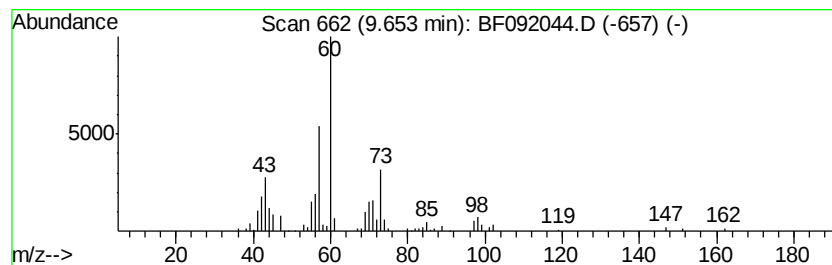
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 9

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.65 | 2.01 ng | 217869 | Acenaphthene-d10 | 9.71 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|---------|---|-------------------------------------|-----|---------|--------------|------|
| 1       |   | 1,6-Anhydro-.beta.-D-glucopyrano... | 162 | C6H10O5 | 000498-07-7  | 72   |
| 2       |   | D-Allose                            | 180 | C6H12O6 | 002595-97-3  | 72   |
| 3       |   | Pentanoic acid                      | 102 | C5H10O2 | 000109-52-4  | 40   |
| 4       |   | Heptanoic acid                      | 130 | C7H14O2 | 000111-14-8  | 40   |
| 5       |   | Ethyl .beta.-d-ribose               | 178 | C7H14O5 | 1000126-95-4 | 40   |



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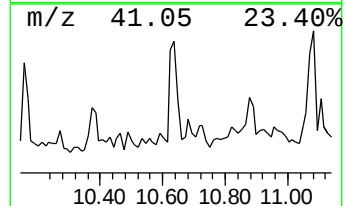
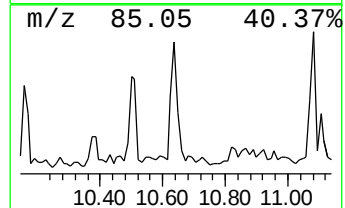
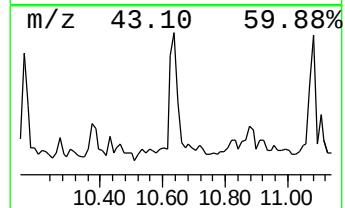
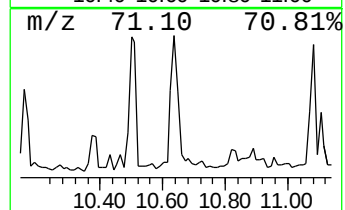
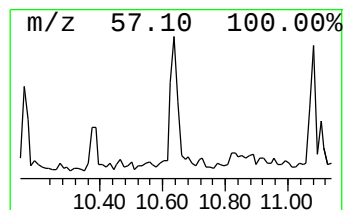
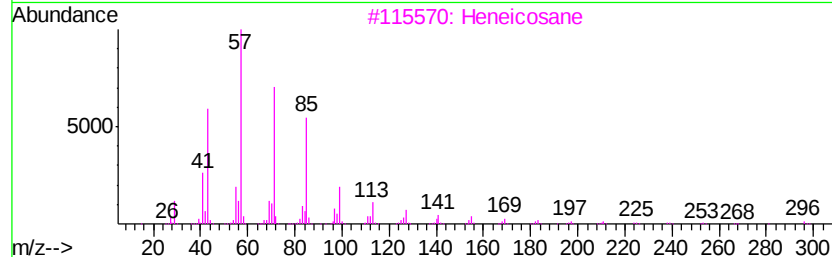
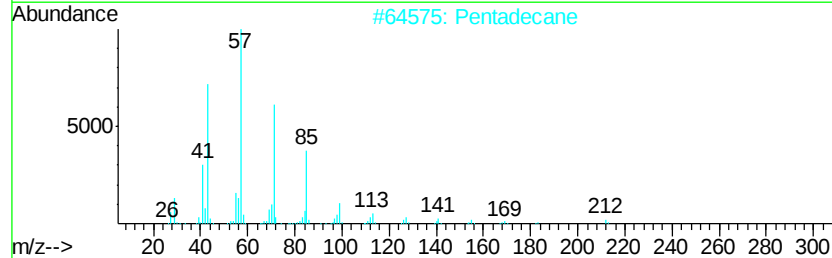
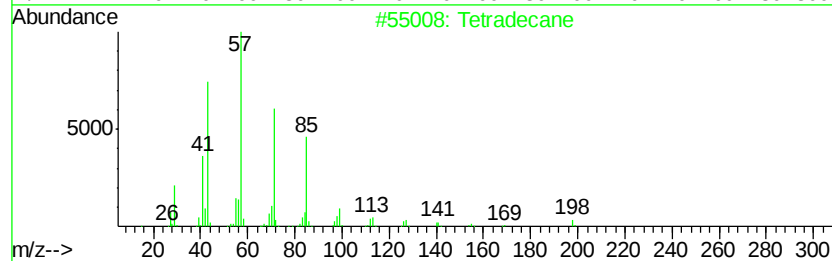
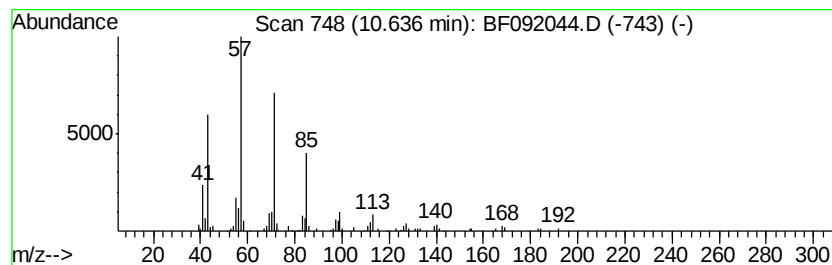
Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Tetradecane Concentration Rank 8

| R.T.    | EstConc | Area         | Relative to ISTD | R.T.           |
|---------|---------|--------------|------------------|----------------|
| 10.64   | 2.07 ng | 238732       | Phenanthrene-d10 | 11.20          |
| Hit# of | 5       | Tentative ID | MW MolForm       | CAS# Qual      |
| 1       |         | Tetradecane  | 198 C14H30       | 000629-59-4 90 |
| 2       |         | Pentadecane  | 212 C15H32       | 000629-62-9 90 |
| 3       |         | Heneicosane  | 296 C21H44       | 000629-94-7 90 |
| 4       |         | Eicosane     | 282 C20H42       | 000112-95-8 90 |
| 5       |         | Hexadecane   | 226 C16H34       | 000544-76-3 90 |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF123016\  
Data File : BF092044.D  
Acq On : 30 Dec 2016 14:01  
Operator : UM/SJ  
Sample : H6262-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

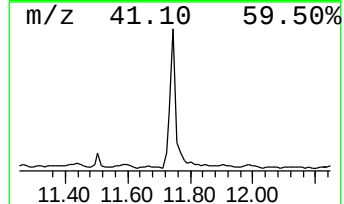
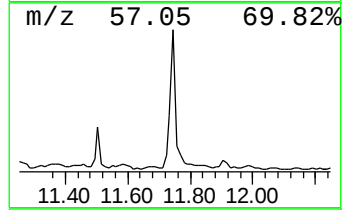
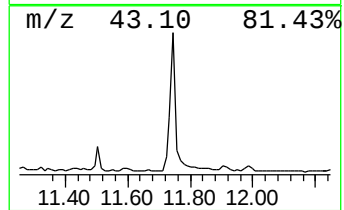
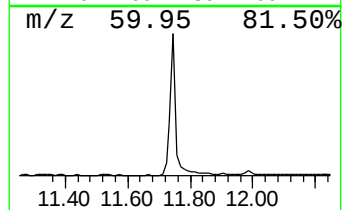
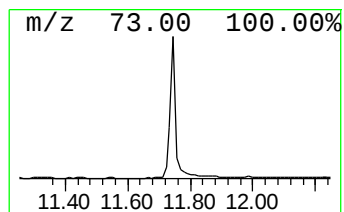
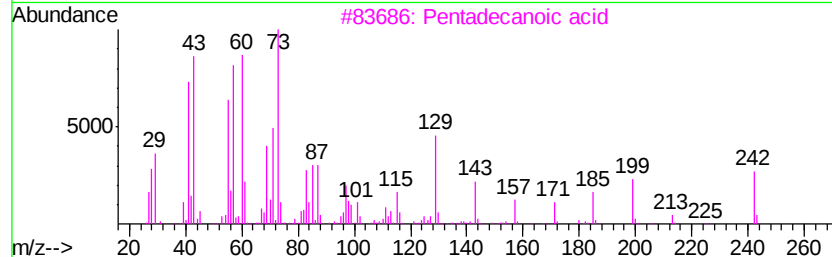
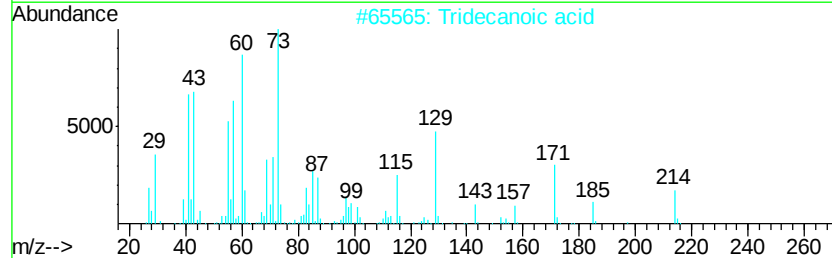
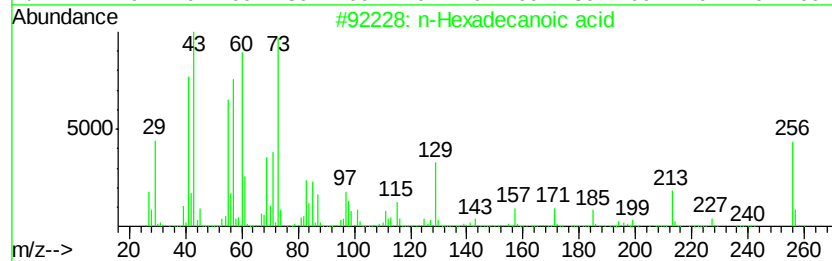
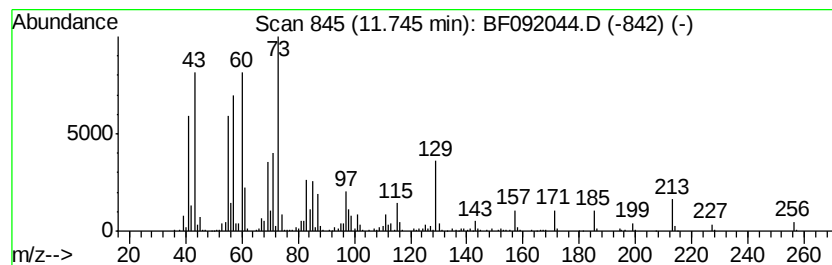
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc  | Area    | Relative to ISTD | R.T.  |
|-------|----------|---------|------------------|-------|
| 11.75 | 11.32 ng | 1305780 | Phenanthrene-d10 | 11.20 |

| Hit# | of | Tentative ID                      | MW  | MolForm  | CAS#        | Qual |
|------|----|-----------------------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid               | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    | Tridecanoic acid                  | 214 | C13H26O2 | 000638-53-9 | 91   |
| 3    |    | Pentadecanoic acid                | 242 | C15H30O2 | 001002-84-2 | 83   |
| 4    |    | Tetradecanoic acid                | 228 | C14H28O2 | 000544-63-8 | 80   |
| 5    |    | Estra-1,3,5(10)-trien-17.beta.-ol | 256 | C18H24O  | 002529-64-8 | 25   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF123016\  
Data File : BF092044.D  
Acq On : 30 Dec 2016 14:01  
Operator : UM/SJ  
Sample : H6262-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

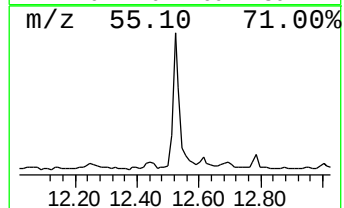
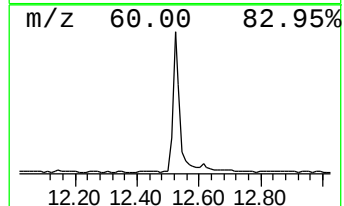
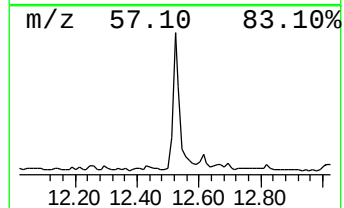
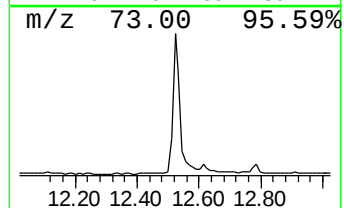
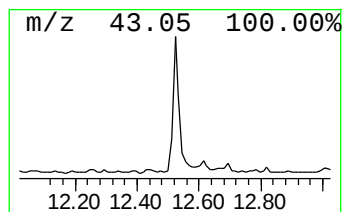
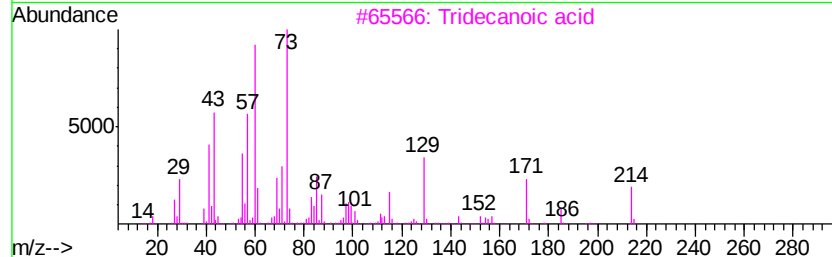
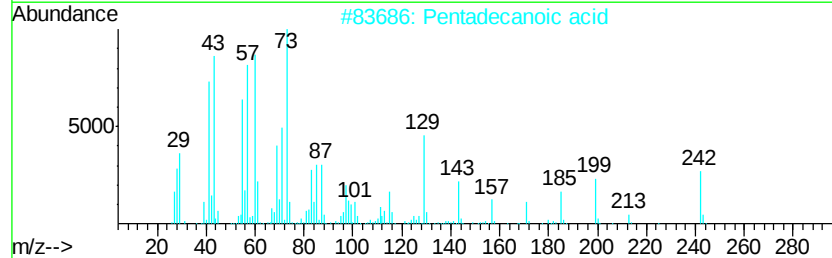
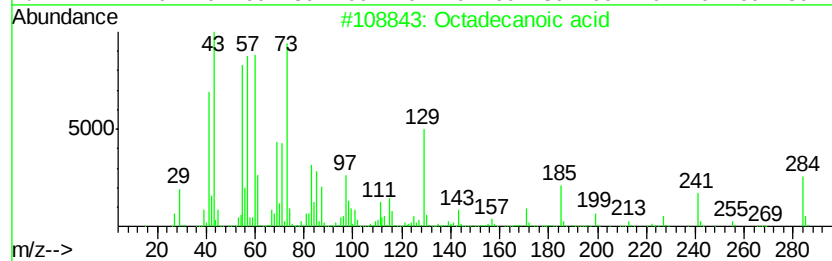
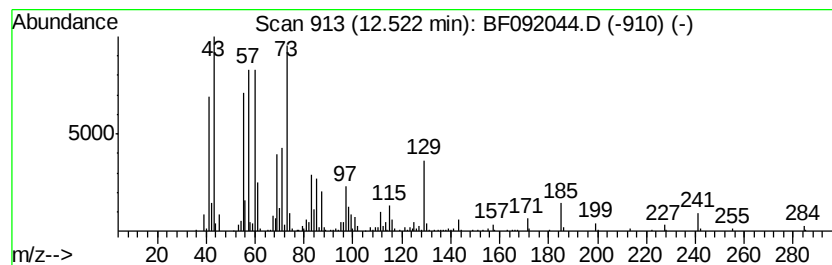
Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Octadecanoic acid Concentration Rank 5

| R.T.    | EstConc | Area                       | Relative to ISTD |          | R.T.        |      |
|---------|---------|----------------------------|------------------|----------|-------------|------|
| 12.52   | 7.28 ng | 818267                     | Chrysene-d12     |          | 13.83       |      |
| Hit# of | 5       | Tentative ID               | MW               | MolForm  | CAS#        | Qual |
| 1       |         | Octadecanoic acid          | 284              | C18H36O2 | 000057-11-4 | 99   |
| 2       |         | Pentadecanoic acid         | 242              | C15H30O2 | 001002-84-2 | 91   |
| 3       |         | Tridecanoic acid           | 214              | C13H26O2 | 000638-53-9 | 72   |
| 4       |         | N-Cyclooct-4-enylacetamide | 167              | C10H17NO | 170952-69-9 | 25   |
| 5       |         | Tridecane                  | 184              | C13H28   | 000629-50-5 | 11   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF123016\  
Data File : BF092044.D  
Acq On : 30 Dec 2016 14:01  
Operator : UM/SJ  
Sample : H6262-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

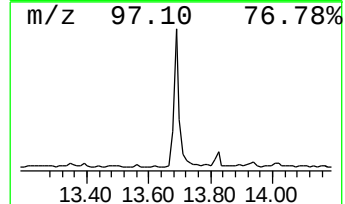
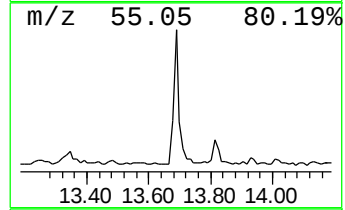
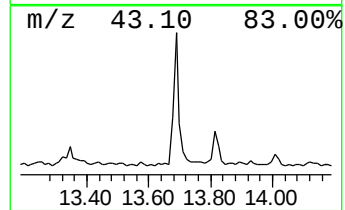
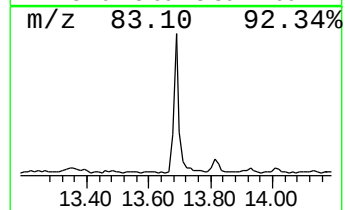
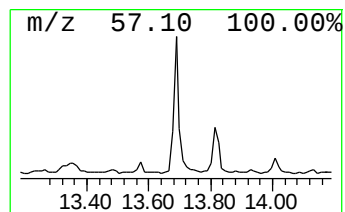
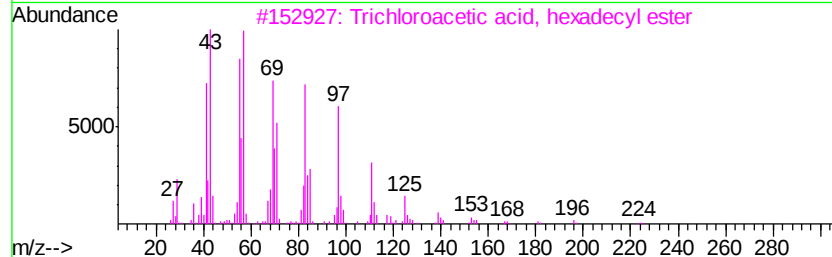
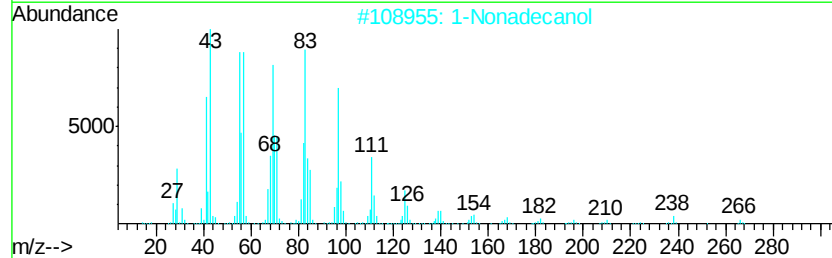
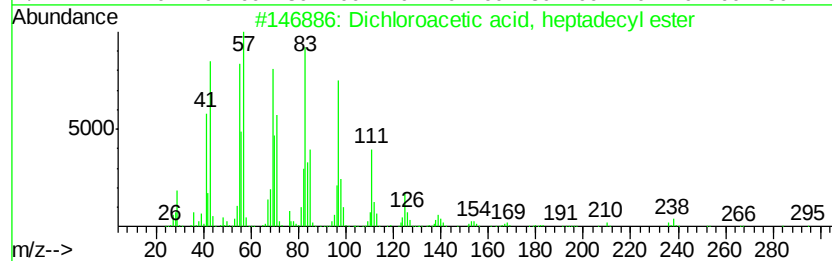
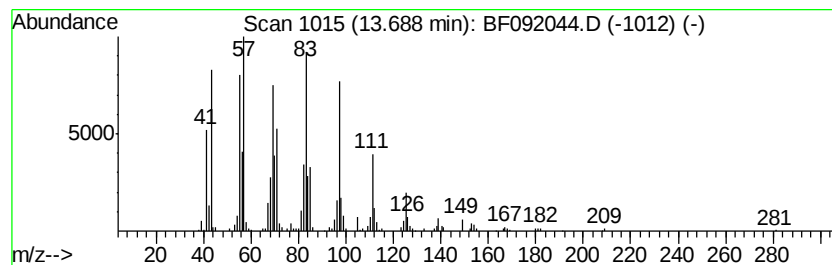
Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 7

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 13.69     | 4.25 ng                             | 477563 | Chrysene-d12     | 13.83        |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | Dichloroacetic acid, heptadecyl ... | 366    | C19H36Cl2O2      | 1000282-98-2 | 95   |
| 2         | 1-Nonadecanol                       | 284    | C19H40O          | 001454-84-8  | 95   |
| 3         | Trichloroacetic acid, hexadecyl ... | 386    | C18H33Cl3O2      | 074339-54-1  | 94   |
| 4         | Heptafluorobutanoic acid, heptad... | 452    | C21H35F7O2       | 1000282-97-3 | 94   |
| 5         | 1-Octadecanol                       | 270    | C18H38O          | 000112-92-5  | 90   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF123016\  
Data File : BF092044.D  
Acq On : 30 Dec 2016 14:01  
Operator : UM/SJ  
Sample : H6262-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
W-4(55-57)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown2.89          | 2.89  | 4.3     | ng    | 271383   | 1                     | 6.68  | 1247930 | 20.0 |
| 2-Pentanone, 4-hy... | 4.83  | 34.1    | ng    | 2126330  | 1                     | 6.68  | 1247930 | 20.0 |
| unknown6.45          | 6.45  | 96.3    | ng    | 6005740  | 1                     | 6.68  | 1247930 | 20.0 |
| 1,6-Anhydro-.beta... | 9.65  | 2.0     | ng    | 217869   | 3                     | 9.71  | 2163330 | 20.0 |
| Tetradecane          | 10.64 | 2.1     | ng    | 238732   | 4                     | 11.20 | 2306950 | 20.0 |
| n-Hexadecanoic acid  | 11.75 | 11.3    | ng    | 1305780  | 4                     | 11.20 | 2306950 | 20.0 |
| Octadecanoic acid    | 12.52 | 7.3     | ng    | 818267   | 5                     | 13.83 | 2248690 | 20.0 |
| Dichloroacetic ac... | 13.69 | 4.3     | ng    | 477563   | 5                     | 13.83 | 2248690 | 20.0 |